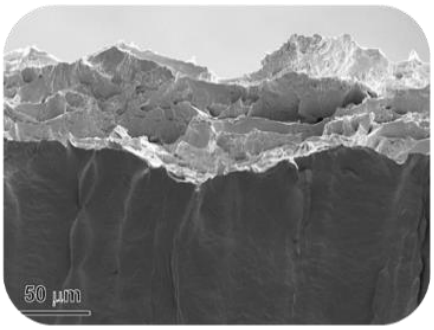
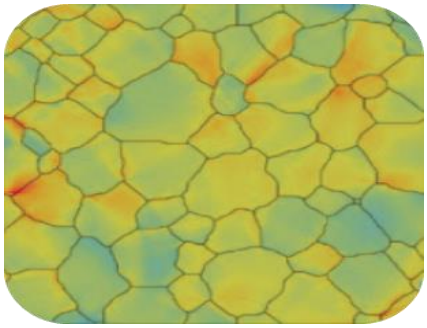
Predicting Performance Margins (PPM)

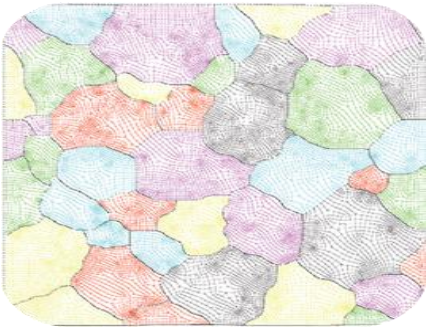
Developing a stochastic framework to better quantify the effects of material variability on performance margins



Oblique 45° tilted image of a fracture surface and a deformed surface of a tensile bar.



von Mises stress distributions in a 79-grain, randomly textured Mo polycrystal in tension and compression calculated by the polycrystal plasticity finite element model.



Model microstructure of molybdenum polycrystal with 64 grains - Finite element mesh

Issue

One of the challenges at Sandia National Laboratories is addressing the issue of predictively connecting the macroscopic properties of metals to their micro- and nanostructure. While this issue may seem straightforward, it is anything but trivial. Materials are intrinsically inhomogeneous, but the relationship between microstructural variability and resulting properties is often unknown.

Approach

PPM is comprised of a group of multidisciplinary staff, post-docs, and university collaborators that are dedicated to address major material science gaps in nuclear weapons mission. Staff from different Centers actively seek science-based, probabilistic underpinning that link material variability to material performance. These include Material Science, Engineering Science, Physical, Chemical, and Nanoscience in both Sandia New Mexico and Sandia California.

Current PPM effort focuses on development of tools and insight towards ensuring the mechanical safety of welded components in our stockpile. This is intended to be a bellwether program where the core theme of materials variability can expand into many other topics from glass/ceramic materials failure to polymer aging to electrical contact tribology.

Capabilities

PPM not only relies on the multidisciplinary expertise and skills across different centers, it also leverages Sandia's existing world-class capabilities in experimental and computational science.

Advanced characterization and testing–

- 3D microscopy
- Focused Ion Beam (FIB)
- Tomography
- Digital image correlation quantitative nano/microstructural scale deformation
- Multi-axial weld test capabilities

Modeling and simulation –

- Material constitutive relations,
- Quantum and atomistic simulations
- Statistical reduced order models
- Homogenization
- Mesoscale material mechanics

Staff Development

PPM is committed to develop early and mid-career staff in order to sustain material science expertise to solve our existing and upcoming NW material challenges. Annual reviews are conducted with both Technical Advisory and Customer Advisory committees to ensure progress and impact to the NW community.

Project Organization

- **Task 1:** Nanoscale framework for crack initiation and growth in Ta and Ta alloys.
- **Task 2:** Microscale effects of defect fields in Ta and Ta alloys.
- **Task 3:** Connecting microstructural variability to performance margins in structural metals.

University Collaborations

- Cornell University
- Drexel University
- Michigan State University
- University of Connecticut
- University of Texas, Austin

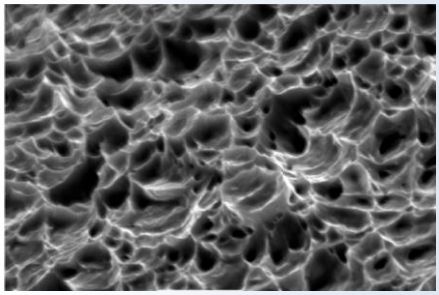
Non-nuclear Material Applications

PPM serves as a prototype extendable to other important material science areas. Building a material science foundation enhances Sandia's agility and responsiveness for future mission needs. PPM demonstrates how different communities collaborate to address recurring non-nuclear materials concerns and to provide critical materials support for our Stockpile.

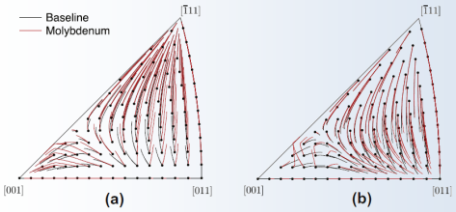
Pertinent areas beyond weld reliability include:

- Glass-to-metal seals failure
- Glass-ceramic to metal seals failure
- Interfacial contact tribology
- Reliable braze and solder joints
- Aging degradation of foams and polymers

Journal Publications

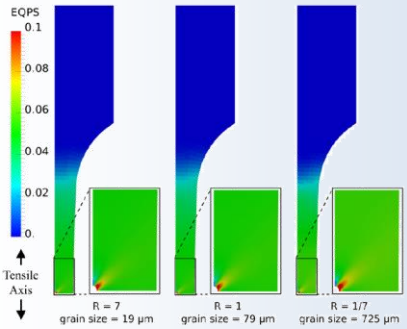


"The Morphology of Tensile Failure in Tantalum", B.L. Boyce, et. Al., Metallurgical and Materials Transactions A. 2012



"Incorporating Atomistic Data of Lattice Friction into BCC Crystal Plasticity Models", C.R. Weinberger, et al., International Journal of Plasticity, 37 (2012) 16-30.

"Quantitative Characterization of Porosity in Laser Welds of Stainless Steel," J.D. Madison, Scripta Materialia, 67 (2012) 783-786.



"The Effect of Grain Size on Local Deformation Near a Void-Like Stress Concentration," J.D. Caroll, et al., International Journal of Plasticity, 39 (2012) 46-60.

For more information please contact:

Amy Sun, Program Manager, acsun@sandia.gov
Brad Boyce, Principal Investigator, blboyce@sandia.gov
Corbett Battaile, Principal Investigator, ccbatta@sandia.gov

U.S. DEPARTMENT OF ENERGY | NNSA National Nuclear Security Administration

Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholl Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC0